Structures and Electronic Properties of Adsorbates on the Si(001) Surface Studied by Photoelectron-Diffraction and-Spectroscopy(Abstracts of Doctoral Dissertations,Annual Report (from April 1996 to March 1997))

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Several technologically and scientifically important adsorbate systems on the Si(001) surface have been studied in detail to reveal their surface geometric and electronic structures. Adsorption of group III elements of Al and In on Si(001) was extensively studied by photoelectron spectroscopy for valence and core electrons and by photoelectron diffraction. Adsorbate system of a group-IV element of Ge on Si(001) was studied by Auger electron diffraction.

(1) For the initial growth of Al and In adsorption on Si(001)

Low energy electron diffraction and X-ray photoelectron spectroscopy studies revealed several new surface phases such as 2x1+streaks-Al, 2x5-Al, 2x3-In and 2x3-In for submonolayer Al and In adsorption on Si(001), which establish a general 2 dimensional growth mode of group-III adsorption on Si(001). Investigations by core-level photoelectron spectroscopy and angle-resolved photoelectron spectroscopy indicate the existence of interfacial reaction for Al adsorption on Si(001) for the first time in contrast to non-reactive growth of In on Si(001).

(2) For the surface structures of In adsorption Si(001)

Of several In-adsorption induced phases on Si(001), two most important well-ordered phases of 2x2-In and 2x3-In were studied in detail by X-ray photoelectron diffraction and Auger electron diffraction with single scattering cluster analyses, which have unambiguously determined the In dimer orientation for both phases to be parallel to the Si surface dimers. The new technique of low energy photoelectron diffraction using synchrotron radiation was applied to the 2x2-, 2x3- and 4x3-In surfaces. For the photoelectron diffraction results of 2x2-In, full multiple scattering cluster analyses were performed, which determined the detailed structural parameters of In dimers. The local structure sensitivity of low energy photoelectron diffraction was confirmed by comparing the photoelectron diffraction results of several different surface structures.

Large anisotropies of spin-orbit branching ratio of In 4d core level were observed for the first time, whose origin was identified by extensive hν-dependent photoelectron diffraction measurements. High-resolution core-level photoelectron spectroscopy using synchrotron radiation investigation for the 2x2- and 2x3-In surfaces revealed the symmetrization of Si dimers bonded to In for both surfaces and buckling of bare Si dimers not bonded to In on the 2x3-In surface. Similar study for the 4x3-In surface suggests several properties of the unknown structure of this surface.

(3) For the surface electronic structures of Al and In adsorptiion on Si(001)

Polarization-dependent angle-resolved photoelectron spectroscopy with synchrotron radiation was applied to the two well-ordered surfaces of single-domain Si(001)2x2-Al and -In to find five surface electronic states common to the two phases. The origins of the five states were clearly identified as the dimer-bond and back-bond surface states of the metal adsorbate dimers. Similar angle-resolved photoelectron spectroscopy study was also done for a single-domain Si(001)2x3-In surface to reveal six surface states which are identified as the dangling-bond surface state of the bare Si dimers and the dimer-bond and back-bond surface states of the In dimers.

(4) For the interface structures of Ge adsorption on Si(001)

An Auger electron diffraction study for monolayer Ge on Si(001) clearly indicated a strong interfacial intermixing of Ge with Si. This intermixing was found to lead to a stable substitutional interface alloy phase after annealing at 500~600 °C. The uniqueness of this work is on the fact that the surface electronic structure and surface geometric structures of the group-III metal adsorption on Si(001) are studied together in a very systematic fashion to give a comprehensive understanding of these systems. In addition, a very new technique of low energy PED using synchrotron radiation was tried successfully to give quantitative information on the surface geometric structures. For further investigations, the structures of the higher temperature phases of Al and In adsorption on Si(001), for instance 4x3-In, should be studied in more detail. The intermixing of Ge on Si(001) also deserve further investigation to clarify the mechanism and possible ordering of interfacial alloying. Detailed surface electronic structure study is also required for monolayer Ge on Si(001). The new tool of low energy PED is expected to be applied to wider variety of surfaces, for which developments for an efficient data taking and efficient and reliable MSC simulations should be done.